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17:45 **UNDERSTAND THE IMPORTANCE OF MOLECULAR ORGANIZATION AT POLYMER-POLYMER INTERFACES IN EXCITONIC SOLAR CELLS**

Authors : Helena M. G. Correia, Hélder M. C. Barbosa, Luís Marques, Marta M. D. Ramos
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Resume : To improve the efficiency of organic solar cells is necessary, for instance, to increase the open-circuit voltage or increase sun-light absorption by covering complementary regions of the solar spectrum. This can be achieved by using a donor-acceptor system composed of two polymers. The versatility of these materials has the advantage of enabling the control of morphology at nanoscale, and thus the design of an adequate interface to improve the device efficiency, using for instance nanoimprint lithography. However, proper control of the molecular organization of both polymers at polymer-polymer interface is difficult and strongly depends on the experimental conditions used. Polymer chains can present different conformations relative to the interface, creating different conjugated strand arrangements whose disorder degree can affect energy and charge transfer. Thus, understanding this effect is of utmost importance to improve the efficiency of excitonic solar cells. In this work we present a Monte Carlo model that uses a proper description of polymer-polymer interface nanomorpholy and considers the main physical processes that mediate excitons and charges dynamics. Our results show that the amount of charge extracted from the interface is sensible to polymer strand orientation and to the presence of the diffusive layer formed by the mixture of both polymers.

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UNDERSTAND THE IMPORTANCE OF MOLECULAR ORGANIZATION AT POLYMER-POLYMER INTERFACES IN EXCITONIC SOLAR CELLS

Universidade do Minho
Escola de Ciências

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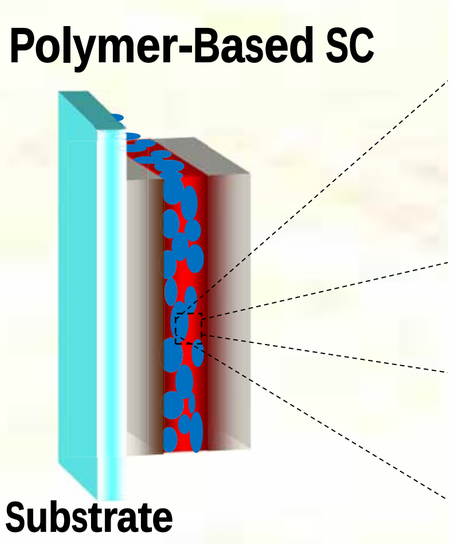
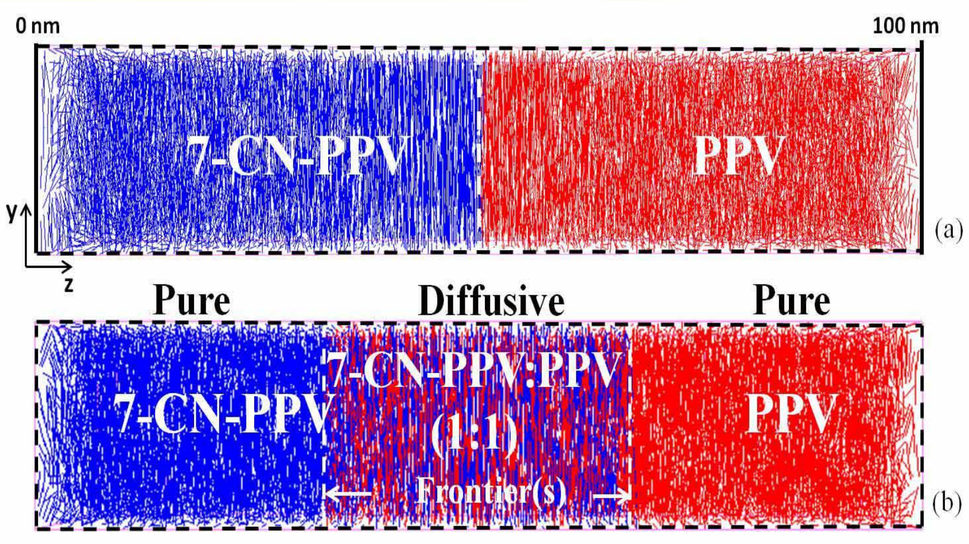
To improve the efficiency of organic solar cells is necessary, for instance, to increase the open-circuit voltage or increase sun-light absorption by covering complementary regions of the solar spectrum. This can be achieved by using a donor-acceptor system composed of two polymers. The versatility of these materials has the advantage of enabling the control of morphology at nanoscale, and thus the design of an adequate interface to improve the device efficiency, using for instance nanoimprint lithography. However, proper control of the molecular organization of both polymers at polymer-polymer interface is difficult and strongly depends on the experimental conditions used. Thus, understanding this effect is of utmost importance to improve the efficiency of excitonic solar cells

MESOSCOPIC MODEL

Systems Used To Model Different Polymer-Polymer Interfaces





Optoeletronic Processes Considered

Exciton Formation

Exciton Decay — **Exciton Diffusion**

Exciton Dissociation

Charge Recombination — **Charge Transport**

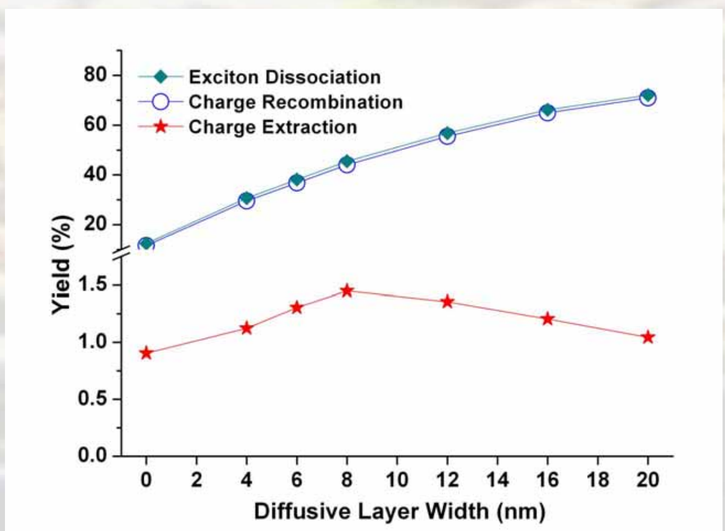
PHOTO code (based on a Monte Carlo method) was used to simulate exciton migration in bilayer polymer networks with different morphologies and diffusive interfaces width. A detaild description of the model can be found in Correia, HMG , et. al., Comput. Mater. Sci. 75 (2013) 18-23.

RESULTS AND CONCLUSION

•The presence of a diffusive interface leads to an increase on exciton quenching when compared to the sharp interface.

• The increase of the diffusive layer thickness increases exciton quenching due to an interpenetration of strands of both polymers, creating a mesh of donor-acceptor sites where excitons can easily dissociate.

•The increase of exciton dissociation is followed by an increase of charge recombination, and the difference between these two leads to a small yield of charge generation at the polymer-polymer with a maximum for a diffusive layer width of 8 nm.



Diffusive	Pristine Layers				Diffusive Layer				Pristine/Diffusive Interfaces			
Layer Thickness	Exc.	Dec.	Diss.	Rec.	Exc.	Dec.	Diss.	Rec.	Exc.	Dec.	Diss.	Rec.
0	94.36	87.37	0.03	6.47	0.00	0.00	0.00	0.00	5.64	0.01	12.37	4.96
4	79.31	69.16	0.00	5.22	10.20	0.00	14.40	14.52	10.49	0.03	16.18	9.74
6	71.30	61.66	0.00	5.18	19.31	0.00	21.74	22.45	9.39	0.05	16.37	9.20
8	63.89	54.37	0.03	5.28	27.34	0.01	30.27	30.60	8.77	0.00	15.15	8.13
12	50.80	43.08	0.00	4.13	41.40	0.02	44.38	44.10	7.80	0.00	12.37	7.18
16	40.08	33.73	0.00	3.54	52.80	0.06	55.38	55.22	7.12	0.00	10.71	6.11
20	32.74	27.45	0.00	2.92	61.64	0.26	62.88	62.85	5.62	0.21	9.09	5.11

• For all diffusive layer thicknesses, the large majority of the excitons created within the diffusive layer and within the pristine/diffusive interface dissociate.

• Part of the excitons dissociated in diffusive regions are created on the neighbour regions.

• Almost all excitons dissociated within the diffusive layer recombine.

• The charge generation at the interface is much higher than the charge collected at the electrodes due to the large amount of recombination taking place within the pristine layers near those interfaces.

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